# Diffusion processes in discontinuous media: numerical algorithms and benchmark tests

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*Workshop* Validation approaches for multiscale porous media models

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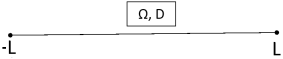
# Outline

1D Diffusion problem

Constant time steps SBM algorithms

Benchmark test cases

# 1D Diffusion problem




$$\begin{cases} \partial_t f(t,y) = \partial_y \left( D(y) \partial_y f(t,y) \right), \\ f(t,\cdot) \xrightarrow[t \to 0]{\text{weakly}} \nu, \\ \textbf{For reflecting BC at } -L \textbf{ and } L\textbf{:}\ D(-L)\partial_y f(t,-L) = D(L)\partial_y f(t,L) = 0, \\ \textbf{For periodic BC:}\ f(t,-L) = f(t,L), \\ \textbf{For reflecting BC at } -L \textbf{ and absorbing BC at } L\textbf{:}\ \begin{cases} D(-L)\partial_y f(t,-L) = 0 \\ f(t,L) = 0 \end{cases} \end{cases}.$$

with $D$ the diffusion coefficient, assumed homogeneous in time.

Motivation: to solve this problem using particle tracking techniques.

Settings:

- The particles are initially distributed according to the measure $\nu$,
- At time t, they are distributed with the density $f(t,\cdot)$,
- The positions of the particles are defined by the paths of **a stochastic process** $(X_t)_{t \geq 0}$ on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$,
- Linear equation $\Rightarrow$ **the particles move independently**.

# Kolmogorov Forward equation

## Approximation of $(X_t)_{t\geq 0}$

- Markov property $\Rightarrow$ Simulate, for $t > s$, $X_t$ when $X_s = x$ is known.

The density transition function $\mathfrak{q}$: Diffusivity is homogeneous in time $\Rightarrow$ the density $y \to \mathfrak{q}(t,x,y)$ of $X_{s+t}$ given $X_s = x$ is solution to the *Fokker-Planck* (or *Kolmogorov forward*) equation:

$$\begin{cases} \partial_t \mathfrak{q}(t,x,y) = \partial_y(D(y)\partial_y \mathfrak{q}(t,x,y)), \\ \mathfrak{q}(t,x,y) \xrightarrow[t\to 0]{\text{weakly}} \delta_x(y), \\ \mathfrak{q}(t,x,\cdot) \text{ satisfies absorbing, reflecting or periodic BC.} \end{cases}$$

$\mathfrak{q}$ is called the *fundamental solution* (or *Green function*).

The density $f(t,y)$ is then equal to

$$f(t,y) = \int_{-L}^{L} \nu(\,\mathrm{d}x)\mathfrak{q}(t,x,y).$$

## Symmetry property

- If the BC at $-L$ is the same as the BC at $L$, then $\mathfrak{q}(t,x,y) = \mathfrak{q}(t,y,x)$ for any $t > 0$ and $x, y \in [-L, L]$.

# Case of an infinite medium:

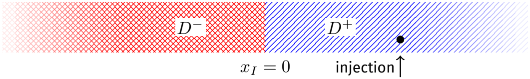
## Constant diffusion coefficient:

- If $D = 1/2$, the stochastic process $X$ is the *Brownian motion* and $\mathfrak{q}(t,x,y)$ is the Gaussian kernel:

$$\mathfrak{g}(t, y-x) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{(x-y)^2}{2t}\right).$$

## Piecewise constant diffusion coefficient:

- With $D(x) = D^+$ if $x \geq 0$ and $D^-$ if $x < 0$,



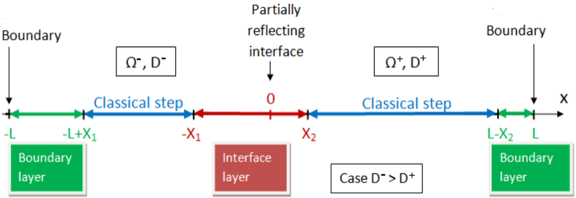

the density transition function of the process X is

$$\mathfrak{q}(t,x,y) = \frac{1}{\sqrt{2D(y)}} \mathfrak{p}_\theta\left(t, \frac{x}{\sqrt{2D(x)}}, \frac{y}{\sqrt{2D(y)}}\right), \quad \text{with: } \theta = \frac{\sqrt{D^+} - \sqrt{D^-}}{\sqrt{D^+} + \sqrt{D^-}},$$

and $\mathfrak{p}_\theta(t,x,y)$ the density transition function of the **Skew Brownian Motion (SBM)** of parameter $\theta$ defined by

$$\mathfrak{p}_\theta(t,x,y) = \mathfrak{g}(t, y-x) + \text{sgn}(y)\theta\mathfrak{g}(t, |y| + |x|).$$

# Case of a finite medium when $D$ is discontinuous




Interface layer $[-X_1, X_2]$ with $X_1 = d_\alpha\sqrt{2\,D^-\,dt}$ and $X_2 = d_\alpha\sqrt{2\,D^+\,dt}$, with $d_\alpha = 4$ so that if $x \notin [-X_1, X_2]$, the next step has very small chance (0.006%) to reach the interface layer.

Outside the interface layer and outside the boundary layers: classical step

$X(t+dt) = x + \xi c_\alpha \sqrt{2\,D^-\,dt}$ on the left $x \in [-L + X_1, -X_1]$
$X(t+dt) = x + \xi c_\alpha \sqrt{2\,D^+\,dt}$ on the right $x \in [X_2, L - X_2]$

Inside the interface layer Scaling: $\Phi(x) = \frac{x}{\sqrt{2D(x)}}$

$X(t+dt) = \Phi^{-1}(Y(dt))$ with $x \in [-X_1, X_2]$, with $Y(dt)$ a Skew Brownian motion with parameter $\theta$, at time $dt$, starting from $Y(0) = \Phi(x)$

# Inside the interface layer: algorithms with constant time steps

## General principle:

**Data:** Starting position $X_t$ at time $t$, a time step $dt$ and a diffusion coefficient $D$.
**Result:** The position $X_{t+dt}$ at time $t+dt$ of the particle.
**Algorithm:**

1. **Scaling:** Let $Y_t = \dfrac{X_t}{\sqrt{2D(X_t)}}$. $Y_t$ is a SBM of parameter $\theta = \dfrac{\sqrt{D^+}-\sqrt{D^-}}{\sqrt{D^+}+\sqrt{D^-}}$
2. **SBM scheme:** Compute $Y_{t+dt}$ using the constant time steps scheme of your choice
3. **New position:** $X_{t+dt} = \sqrt{2D(Y_{t+dt})}Y_{t+dt}$ (Scaling)

## Some SBM schemes:

- `Uffink`: approximation method proposed by Uffink, PhD thesis, 1990
  $\Rightarrow$ single step, Uniform steps $\xi \sim \mathcal{U}(-1,1)$, $c_\alpha = \sqrt{3}$
- `HMYLA`: approximation method proposed by Hoteit *et al.*, Math. Geology, 2002
  $\Rightarrow$ two-steps, Uniform steps, $\xi \sim \mathcal{U}(-1,1)$, $c_\alpha = \sqrt{3}$
- `SBM`: exact density-based algorithm proposed by Lejay & Pichot, JCP, 2014
  $\Rightarrow$ two-steps, Gaussian steps $\xi \sim \mathcal{N}(0,1)$, $c_\alpha = 1$
- SBMlin: exact density-based algorithm with a linear interpolation for the time in case of crossing, Lejay & Pichot, JCP, 2014
  $\Rightarrow$ two-steps, Gaussian steps $\xi \sim \mathcal{N}(0,1)$, $c_\alpha = 1$

# One step method - Method 1: Uffink, PhD thesis, 1990

**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

Compute $H1 = \sqrt{6D^- dt}$ and $H2 = \sqrt{6D^+ dt}$;
**if** $x + H1 \leq 0$ **then**
  /∗the interface is not crossed: uniform step;
  $X_{t+dt} = x + H1\,\mathcal{U}(-1, 1)$;
**else**
  /∗the interface is crossed: biased step;
  Compute special points and $P_U$: ;
  $xL = x - H1$;
  $xM = -x - H1$;
  $xR = (x + H1) * (H2/H1)$;
  $P_U = \dfrac{1}{2\,H1} * (xM - xL)$ ;
  Generate $U \sim \mathcal{U}([0, 1))$;
  **if** $U \leq P_U$ **then**
    Generate $X_{t+dt} \sim \mathcal{U}([xL, xM])$;
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**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.
Compute $H1 = \sqrt{6D^{-}\,dt}$ and $H2 = \sqrt{6D^{+}dt}$;
**if** $x + H1 \leq 0$ **then**
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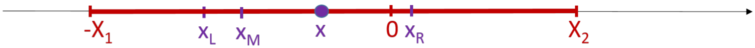

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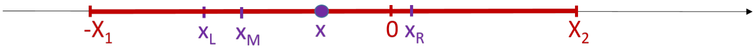

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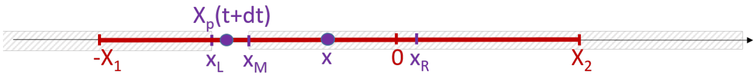

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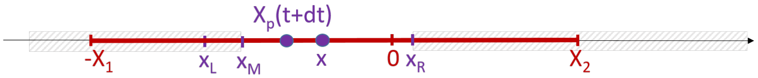
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

```
Compute H1 = sqrt(6 D^- dt) and H2 = sqrt(6 D^+ dt);
if x + H1 <= 0 then
    /*the interface is not crossed: uniform step;
    X_{t+dt} = x + H1 U(-1, 1);
else
    /*the interface is crossed: biased step;
    Compute special points and P_U: ;
    xL = x - H1;
    xM = -x - H1;
    xR = (x + H1) * (H2/H1);
    P_U = 1/(2 H1) * (xM - xL) ;
    Generate U ~ U([0, 1));
    if U <= P_U then
        Generate X_{t+dt} ~ U([xL, xM]);
    else
        Generate X_{t+dt} ~ U([xM, xR]);
    end
end
return X(t + dt);
```

Where: $H1 = \sqrt{6D^- dt}$, $H2 = \sqrt{6D^+ dt}$, $X_{t+dt} = x + H1\,\mathcal{U}(-1,1)$, $P_U = \frac{1}{2\,H1} * (xM - xL)$, $U \sim \mathcal{U}([0,1))$, $X_{t+dt} \sim \mathcal{U}([xL, xM])$, $X_{t+dt} \sim \mathcal{U}([xM, xR])$.



# Two steps methods - Numerical simulation of the first hitting time $\tau$

## Brownian bridge

The Brownian path $(W_t)_{t\in[0,dt]}$ between $x = W_0$ and $y = W_{dt}$ is the Brownian bridge.
When $x < 0$, there are two cases: $y > 0$ and $y < 0$.

## When the bridge crosses the interface: $x < 0$ and $y > 0$

The path hits the interface at time $\tau$ given by
$\tau = dt\xi/(1+\xi)$ with $\xi \sim \mathcal{IG}(-x/y, x^2/dt)$, inverse Gaussian distribution
The time $\tau$ can be approximated by a linear interpolation when $dt$ is small:
$\tau \simeq dt|x|/(|x| + |y|)$

## When the bridge does not cross the interface: $x < 0$ and $y < 0$

The path may cross the interface with the probability $P_c = \exp(-2xy/dt)$
If such, again, the first hitting time is given by an inverse Gaussian distribution
Else it does not cross the interface and $\tau = dt$
The time $\tau$ can be approximated by $\tau = dt$ because the probability $P_c$ is small

# Two steps method - Method 2: HMYLA, Hoteit *et al.*, Math. Geology, 2002

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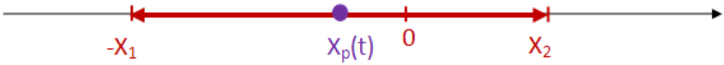
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

Generate $Y \sim \sqrt{6D^- dt}\,\mathcal{U}(-1,1)$;
**if** $Y \leq 0$ **then**
  $X_{t+dt} = Y$;
**else**
  Compute $l_0 = |X_t|$ and $l = |Y - X_t|$; $\tau = \frac{l_0}{l} dt$; /* Linear hitting time */
  Move the particle at 0: $X_{t+\tau} = 0$, $dt_2 = dt - \tau$;
  Compute the transmission probability: $P_H = \frac{1-\theta}{2} = \frac{\sqrt{D^-}}{\sqrt{D^+} + \sqrt{D^-}}$;
  Generate $U \sim \mathcal{U}([0,1))$;
  **if** $U \leq P_H$ **then**
    Generate $X_{t+dt} \sim \mathcal{U}([-\sqrt{6\,dt_2\,D^-}, 0])$;
  **else**
    Generate $X_{t+dt} \sim \mathcal{U}([0, \sqrt{6\,dt_2\,D^+}])$;
  **end**
**end**
**return** $X_p(t+dt)$;



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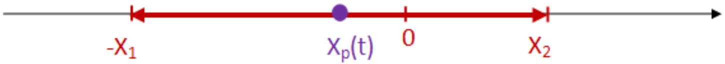

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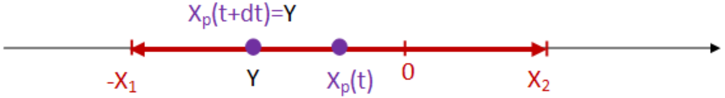

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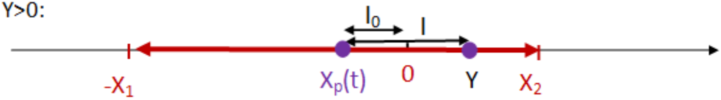
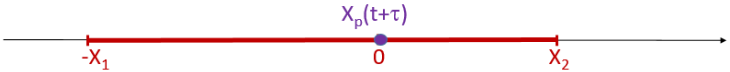
  $X_{t+dt} = \mathrm{Y}$;
**else**
  Compute $l_0 = |X_t|$ and $l = |Y - X_t|$; $\tau = \frac{l_0}{l} dt$; `/* Linear hitting time */`
  Move the particle at 0: $X_{t+\tau} = 0$, $dt_2 = dt - \tau$;
  Compute the transmission probability: $P_H = \frac{1-\theta}{2} = \frac{\sqrt{D^-}}{\sqrt{D^+} + \sqrt{D^-}}$;
  Generate $U \sim \mathcal{U}([0, 1))$;
  **if** $U \leq P_H$ **then**
    Generate $X_{t+dt} \sim \mathcal{U}([-\sqrt{6\, dt_2\, D^-}, 0])$;
  **else**
    Generate $X_{t+dt} \sim \mathcal{U}([0, \sqrt{6\, dt_2\, D^+}])$;
  **end**
**end**
**return** $X_p(t + dt)$;

If Y>0:



# Two steps method - Method 2: HMYLA, Hoteit *et al.*, Math. Geology, 2002

**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.
Generate $Y \sim \sqrt{6D^- \, dt}\,\mathcal{U}(-1, 1)$;
**if** $Y \leq 0$ **then**
    $X_{t+dt} = \mathrm{Y}$;
**else**
    Compute $l_0 = |X_t|$ and $l = |Y - X_t|$; $\tau = \dfrac{l_0}{l}\, dt$; `/* Linear hitting time */`
    Move the particle at 0: $X_{t+\tau} = 0$, $dt_2 = dt - \tau$;
    Compute the transmission probability: $P_H = \dfrac{1-\theta}{2} = \dfrac{\sqrt{D^-}}{\sqrt{D^+} + \sqrt{D^-}}$;
    Generate $U \sim \mathcal{U}([0, 1))$;
    **if** $U \leq P_H$ **then**
        Generate $X_{t+dt} \sim \mathcal{U}([-\sqrt{6\, dt_2\, D^-}, 0])$;
    **else**
        Generate $X_{t+dt} \sim \mathcal{U}([0, \sqrt{6\, dt_2\, D^+}])$;
    **end**
**end**
**return** $X_p(t + dt)$;



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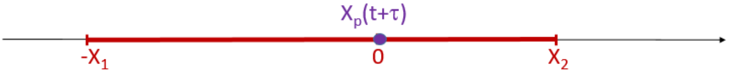
**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

Generate $Y \sim \sqrt{6D^- \, dt}\,\mathcal{U}(-1,1)$;
**if** $Y \le 0$ **then**
  $X_{t+dt} = Y$;
**else**
  Compute $l_0 = |X_t|$ and $l = |Y - X_t|$; $\tau = \frac{l_0}{l}\, dt$; `/* Linear hitting time */`
  Move the particle at 0: $X_{t+\tau} = 0$, $dt_2 = dt - \tau$;
  Compute the transmission probability: $P_H = \frac{1-\theta}{2} = \frac{\sqrt{D^-}}{\sqrt{D^+} + \sqrt{D^-}}$;
  Generate $U \sim \mathcal{U}([0,1))$;
  **if** $U \le P_H$ **then**
    Generate $X_{t+dt} \sim \mathcal{U}([-\sqrt{6\, dt_2\, D^-}, 0])$;
  **else**
    Generate $X_{t+dt} \sim \mathcal{U}([0, \sqrt{6\, dt_2\, D^+}])$;
  **end**
**end**
**return** $X_p(t + dt)$;



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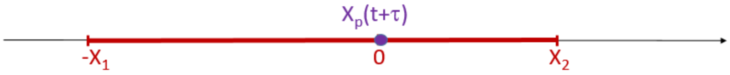
**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

Generate $Y \sim \sqrt{6D^- dt}\,\mathcal{U}(-1,1)$;
**if** $Y \leq 0$ **then**
    $X_{t+dt} = Y$;
**else**
    Compute $l_0 = |X_t|$ and $l = |Y - X_t|$; $\tau = \frac{l_0}{l} dt$; /* Linear hitting time */
    Move the particle at 0: $X_{t+\tau} = 0$, $dt_2 = dt - \tau$;
    Compute the transmission probability: $P_H = \frac{1-\theta}{2} = \frac{\sqrt{D^-}}{\sqrt{D^+} + \sqrt{D^-}}$;
    Generate $U \sim \mathcal{U}([0,1))$;
    **if** $U \leq P_H$ **then**
        Generate $X_{t+dt} \sim \mathcal{U}([-\sqrt{6\,dt_2\,D^-}, 0])$;
    **else**
        Generate $X_{t+dt} \sim \mathcal{U}([0, \sqrt{6\,dt_2\,D^+}])$;
    **end**
**end**
**return** $X_p(t + dt)$;

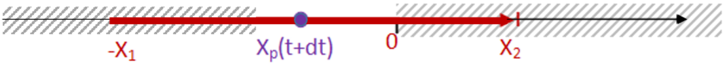


# Two steps method - Method 2: HMYLA, Hoteit *et al.*, Math. Geology, 2002

**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

```
Generate Y ~ sqrt(6D^- dt) U(-1, 1);
if Y ≤ 0 then
    X_{t+dt} = Y;
else
    Compute l_0 = |X_t| and l = |Y - X_t|; τ = (l_0 / l) dt;  /* Linear hitting time */
    Move the particle at 0: X_{t+τ} = 0, dt_2 = dt - τ;
    Compute the transmission probability: P_H = (1 - θ)/2 = sqrt(D^-) / (sqrt(D^+) + sqrt(D^-));
    Generate U ~ U([0, 1));
    if U ≤ P_H then
        Generate X_{t+dt} ~ U([-sqrt(6 dt_2 D^-), 0]);
    else
        Generate X_{t+dt} ~ U([0, sqrt(6 dt_2 D^+)]);
    end
end
return X_p(t + dt);
```

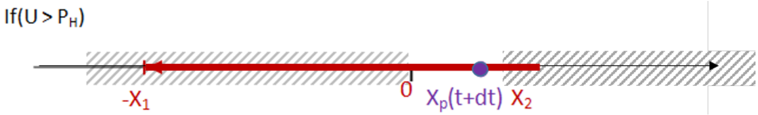
If$(U \leq P_H)$



# Two steps method - Method 2: HMYLA, Hoteit *et al.*, Math. Geology, 2002

**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

Generate $Y \sim \sqrt{6D^- dt}\,\mathcal{U}(-1, 1)$;
**if** $Y \leq 0$ **then**
  $X_{t+dt} = Y$;
**else**
  Compute $l_0 = |X_t|$ and $l = |Y - X_t|$; $\tau = \frac{l_0}{l} dt$; `/* Linear hitting time */`
  Move the particle at 0: $X_{t+\tau} = 0$, $dt_2 = dt - \tau$;
  Compute the transmission probability: $P_H = \frac{1-\theta}{2} = \frac{\sqrt{D^-}}{\sqrt{D^+} + \sqrt{D^-}}$;
  Generate $U \sim \mathcal{U}([0, 1))$;
  **if** $U \leq P_H$ **then**
    Generate $X_{t+dt} \sim \mathcal{U}([-\sqrt{6\, dt_2\, D^-}, 0])$;
  **else**
    Generate $X_{t+dt} \sim \mathcal{U}([0, \sqrt{6\, dt_2\, D^+}])$;
  **end**
**end**
**return** $X_p(t + dt)$;



# Two steps method - Method 3 and 4: SBM and SBMlin, Lejay & Pichot, JCP, 2014

**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

SBM $(\tau, y) \leftarrow$ ExactHittingTime$(t, x, dt, D^-)$;
SBMlin $(\tau, y) \leftarrow$ LinearHittingTimeGS$(t, x, dt, D^-)$);
**if** $\tau < dt$ **then**
  /* A crossing occurred: biased step */
  Generate a random variate $U \in\sim \mathcal{U}(0,1)$;
  Generate a random variate $G_2 \sim \mathcal{N}(0,1)$;
  **if** $U < (1+\theta)/2$ **then**
    **return** $\sqrt{2D^+(dt-\tau)}|G_2|$
  **else**
    **return** $-\sqrt{2D^-(dt-\tau)}|G_2|$
  **end**
**else**
  /* No crossing occurred */
  **return** $y$
**end**

# Two steps method - Method 3 and 4: SBM and SBMlin, Lejay & Pichot, JCP, 2014

**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

SBM $(\tau, y) \leftarrow$ ExactHittingTime$(t, x, dt, D^-)$;

SBMlin $(\tau, y) \leftarrow$ LinearHittingTimeGS$(t, x, dt, D^{-)})$;

**if** $\tau < dt$ **then**

  /* A crossing occurred: biased step */

  Generate a random variate $U \in\sim \mathcal{U}(0, 1)$;

  Generate a random variate $G_2 \sim \mathcal{N}(0, 1)$;

  **if** $U < (1 + \theta)/2$ **then**

    **return** $\sqrt{2D^+(dt - \tau)}|G_2|$

  **else**

    **return** $-\sqrt{2D^-(dt - \tau)}|G_2|$

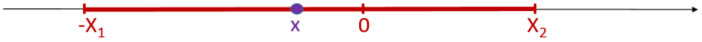
  **end**

**else**

  /* No crossing occurred */

  **return** $y$

**end**



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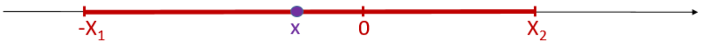
SBM $(\tau, y) \leftarrow$ ExactHittingTime$(t, x, dt, D^-)$;
SBMlin $(\tau, y) \leftarrow$ LinearHittingTimeGS$(t, x, dt, D^-)$);
**if** $\tau < dt$ **then**
  /* A crossing occurred: biased step */
  Generate a random variate $U \in\sim \mathcal{U}(0, 1)$;
  Generate a random variate $G_2 \sim \mathcal{N}(0, 1)$;
  **if** $U < (1 + \theta)/2$ **then**
    **return** $\sqrt{2D^+(dt - \tau)}|G_2|$
  **else**
    **return** $-\sqrt{2D^-(dt - \tau)}|G_2|$
  **end**
**else**
  /* No crossing occurred */
  **return** $y$
**end**



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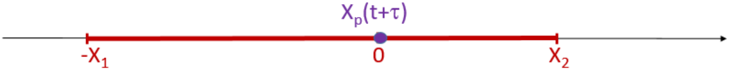
**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.
SBM $(\tau, y) \leftarrow$ ExactHittingTime$(t, x, dt, D^-)$;
SBMlin $(\tau, y) \leftarrow$ LinearHittingTimeGS$(t, x, dt, D^-)$);
**if** $\tau < dt$ **then**
    /* A crossing occurred: biased step */
    Generate a random variate $U \in\sim \mathcal{U}(0, 1)$;
    Generate a random variate $G_2 \sim \mathcal{N}(0, 1)$;
    **if** $U < (1 + \theta)/2$ **then**
        **return** $\sqrt{2D^+(dt - \tau)}|G_2|$
    **else**
        **return** $-\sqrt{2D^-(dt - \tau)}|G_2|$
    **end**
**else**
    /* No crossing occurred */
    **return** $y$
**end**



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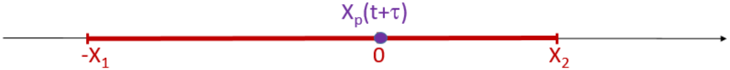
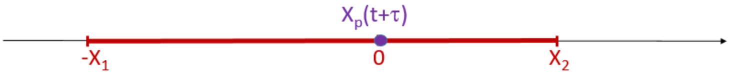
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.
SBM $(\tau, y) \leftarrow \mathrm{ExactHittingTime}(t, x, dt, D^-)$;
SBMlin $(\tau, y) \leftarrow \mathrm{LinearHittingTimeGS}(t, x, dt, D^-)$);
**if** $\tau < dt$ **then**
  /* A crossing occurred: biased step */
  Generate a random variate $U \in\sim \mathcal{U}(0, 1)$;
  Generate a random variate $G_2 \sim \mathcal{N}(0, 1)$;
  **if** $U < (1 + \theta)/2$ **then**
    **return** $\sqrt{2D^+(dt - \tau)}|G_2|$
  **else**
    **return** $-\sqrt{2D^-(dt - \tau)}|G_2|$
  **end**
**else**
  /* No crossing occurred */
  **return** $y$
**end**



# Two steps method - Method 3 and 4: SBM and SBMlin, Lejay & Pichot, JCP, 2014

**Data:** Initial position $X_t = x$, a time $dt > 0$ and interface at 0. Case $x < 0$
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.

```
SBM (τ, y) ← ExactHittingTime(t, x, dt, D⁻);
SBMlin (τ, y) ← LinearHittingTimeGS(t, x, dt, D⁻));
if τ < dt then
    /* A crossing occurred: biased step */
    Generate a random variate U ∈∼ U(0, 1);
    Generate a random variate G₂ ∼ N(0, 1);
    if U < (1 + θ)/2 then
        return √(2D⁺(dt − τ)) |G₂|
    else
        return −√(2D⁻(dt − τ)) |G₂|
    end
else
    /* No crossing occurred */
    return y
end
```



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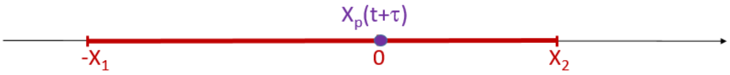
SBMlin $(\tau, y) \leftarrow$ LinearHittingTimeGS$(t, x, dt, D^-)$);
**if** $\tau < dt$ **then**
  /* A crossing occurred: biased step */
  Generate a random variate $U \in\sim \mathcal{U}(0, 1)$;
  Generate a random variate $G_2 \sim \mathcal{N}(0, 1)$;
  **if** $U < (1 + \theta)/2$ **then**
    **return** $\sqrt{2D^+(dt - \tau)}|G_2|$
  **else**
    **return** $-\sqrt{2D^-(dt - \tau)}|G_2|$
  **end**
**else**
  /* No crossing occurred */
  **return** $y$
**end**



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**if** $\tau < dt$ **then**
    /* A crossing occurred: biased step */
    Generate a random variate $U \in\sim \mathcal{U}(0, 1)$;
    Generate a random variate $G_2 \sim \mathcal{N}(0, 1)$;
    **if** $U < (1 + \theta)/2$ **then**
        **return** $\sqrt{2D^+(dt - \tau)}|G_2|$
    **else**
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    **end**
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**if** $\tau < dt$ **then**
  /* A crossing occurred: biased step */
  Generate a random variate $U \in\sim \mathcal{U}(0, 1)$;
  Generate a random variate $G_2 \sim \mathcal{N}(0, 1)$;
  **if** $U < (1 + \theta)/2$ **then**
    **return** $\sqrt{2D^+(dt - \tau)}|G_2|$
  **else**
    **return** $-\sqrt{2D^-(dt - \tau)}|G_2|$
  **end**
**else**
  /* No crossing occurred */
  **return** $y$
**end**

# Two steps method - Method 3 and 4: SBM and SBMlin, Lejay & Pichot, JCP, 2014

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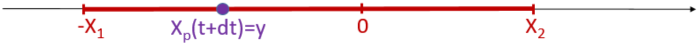
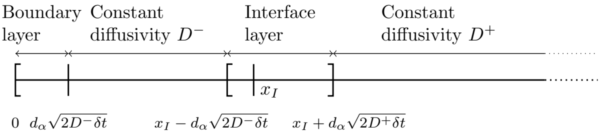
**Result:** Next position $X_{t+dt}$ at time $t + dt$ of the particle.
SBM $(\tau, y) \leftarrow$ ExactHittingTime$(t, x, dt, D^-)$;
SBMlin $(\tau, y) \leftarrow$ LinearHittingTimeGS$(t, x, dt, D^-)$);
**if** $\tau < dt$ **then**
  `/* A crossing occurred: biased step */`
  Generate a random variate $U \in\sim \mathcal{U}(0, 1)$;
  Generate a random variate $G_2 \sim \mathcal{N}(0, 1)$;
  **if** $U < (1 + \theta)/2$ **then**
    **return** $\sqrt{2D^+(dt - \tau)}|G_2|$
  **else**
    **return** $-\sqrt{2D^-(dt - \tau)}|G_2|$
  **end**
**else**
  `/* No crossing occurred */`
  **return** $y$
**end**



# Design of the benchmarks tests

- The tests we proposed are designed **to discriminate between the possible bias and the Monte Carlo error**. They give the fine behavior of schemes and **do not aim at being realistic**. The *bias* is the error induced by the approximation schemes. The smaller, the better.
- A test is ***passed* if one cannot distinguish the bias from the Monte Carlo error**. Otherwise the test *failed*.
- A good benchmark test dedicated to emphasize the bias of schemes must have **a domain size and a time step chosen accordingly** so as to maximize the number of crossing of the interfaces.
- In the benchmark tests, the size of the domain is chosen so that we **can easily test new schemes and change the boundary conditions independently**.
- Invalidating a scheme does not means it should be ruled out. A scheme could be fair enough for computing some macroscopic parameters but not for dealing with microscopic ones.

## Three kinds of zones

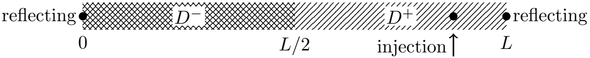


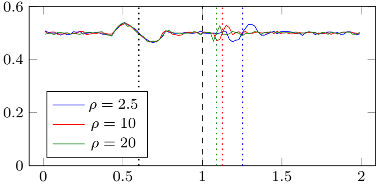

### Algorithms in the boundary layer

- absorbing BC: the hitting time may be computed either exactly or with a linear approximation
- periodic BC: reinject the particle into the medium in a periodic way.
- reflecting BC: perform a reflection around the boundary point.

# Caution: Combination of algorithms

- Since `Uffink` and `HMYLA` rely on uniform approximations, they should be coupled with schemes relying on uniform approximations to avoid bad behavior when the particle is moved from one zone to another.

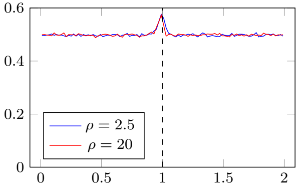


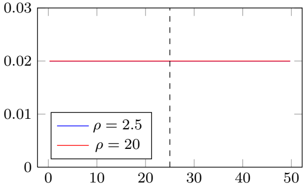

Histograms of the positions of $2 \times 10^6$ particles at time $T = 10$ ($dt = 0.001$) with $L = 2$ for `HMYLA` coupled with `GaussianStep` outside the interface layer for three values of $\rho = \frac{D^-}{D^+}$.

# Parameters settings

- **Number of particles:** Simulate the dynamic of $N$ particles until the final time $T$ is reached. Large number of particles so that the Monte Carlo error, in general of order $\mathrm{O}(N^{-1/2})$, is small. $N$ chosen from $10^5$ to $10 \times 10^6$ particles.
- **Size of the domain, for a given time step:** the input time step $dt$ determines the size of the domain so as to maximize the number of passage through the interface layer by maximizing the relative size of the interface layer within the medium.



(a) Size of the media: 2

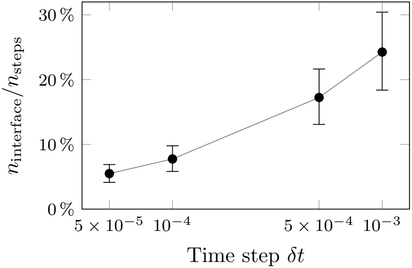


(b) Size of the media: 50

Increasing the size of the domain without changing the time step hides artificially the potential bias of the scheme which appears only when the particle is in the interface layer. Test case with $dt = 0.001$, $T = 10$, Bimaterial medium, `SBMlin`.

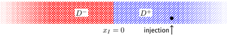
# Parameters settings

- **Time step, for a given domain size:** the time step must be chosen so as to keep a large amount of particles that cross the interface layer. A caution must be observed if the time step is decreased while leaving the medium unchanged.




Mean proportion of steps performed in the interface layer as a function of the time step. Example with a bimaterial medium with reflecting BC and $D^- = 5$, $D^+ = 0.25$ ($\rho = 20$) for `SBM`, $L = 2$ and $x_I = 1$, $T = 10$ and $N = 10{,}000$ particles, initially uniformly distributed.
Remark (not shown): the mean proportion of steps in the interface layer varies from 32 % for $\rho = 2.5$ to 25 % for $\rho = 750$.

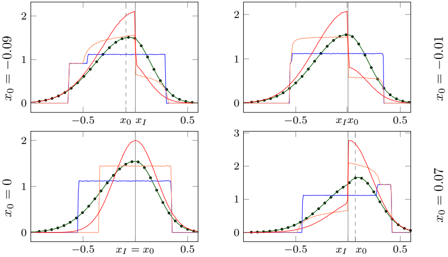
# Benchmark test DENSITIES

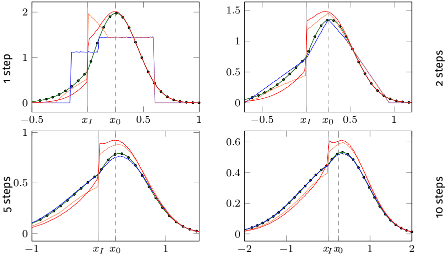



Exact density $q(t, x_0, \cdot)$ (black dots) vs empirical densities

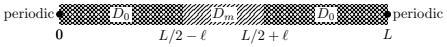
| | |
|---|---|
| SBM | Green |
| Uffink | Blue |
| HMYLA | Coral |
| SBMlin | Red |

$D_- = 5, D_+ = 2,$
$x_I = 0,\ dt = 0.01,$
$N = 10^7$ particles.



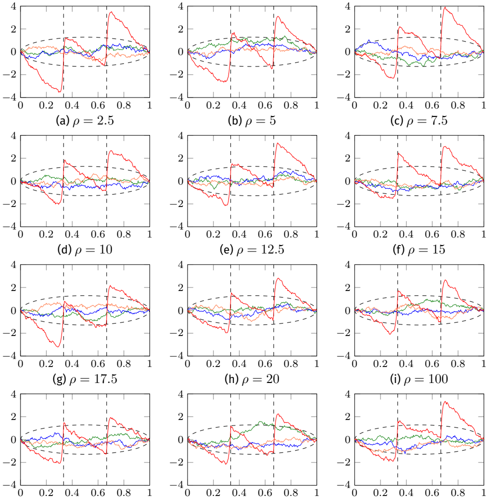
# Benchmark test LAYER




Emp. dist. of particles in stationary regime (≈ uniform)

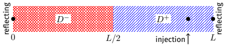
| | |
|---|---|
| `SBM` | Green |
| `Uffink` | Blue |
| `HMYLA` | Coral |
| `SBMlin` | Red |

$\rho = \frac{D_0}{D_m}$, $T = 10$,
$dt = 0.01$, $N = 2x10^6$




(a) $\rho = 2.5$ (b) $\rho = 5$ (c) $\rho = 7.5$
(d) $\rho = 10$ (e) $\rho = 12.5$ (f) $\rho = 15$
(g) $\rho = 17.5$ (h) $\rho = 20$ (i) $\rho = 100$
(j) $\rho = 250$ (k) $\rho = 500$ (l) $\rho = 750$

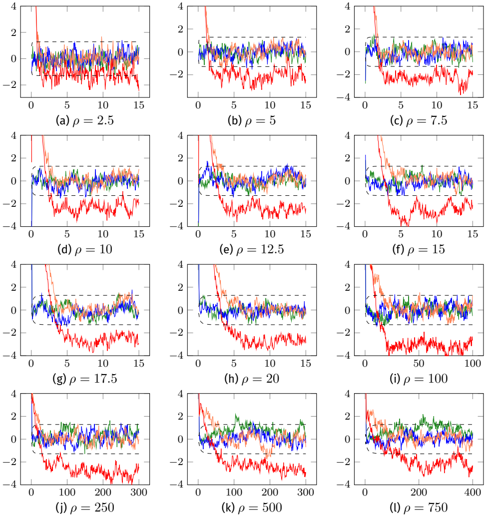
# Benchmark test BIMATERIAL




$t \to \sqrt{N}$(# particles in the right side − theor. value)

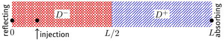
| | |
|---|---|
| SBM | Green |
| Uffink | Blue |
| HMYLA | Coral |
| SBMlin | Red |

$\rho = \frac{D_-}{D_+}$, $D^- = 5$, $L = 2$, $x_0 = 1.5$, $dt = 0.001$, $N = 4x10^6$.



(a) $\rho = 2.5$ (b) $\rho = 5$ (c) $\rho = 7.5$ (d) $\rho = 10$ (e) $\rho = 12.5$ (f) $\rho = 15$ (g) $\rho = 17.5$ (h) $\rho = 20$ (i) $\rho = 100$ (j) $\rho = 250$ (k) $\rho = 500$ (l) $\rho = 750$

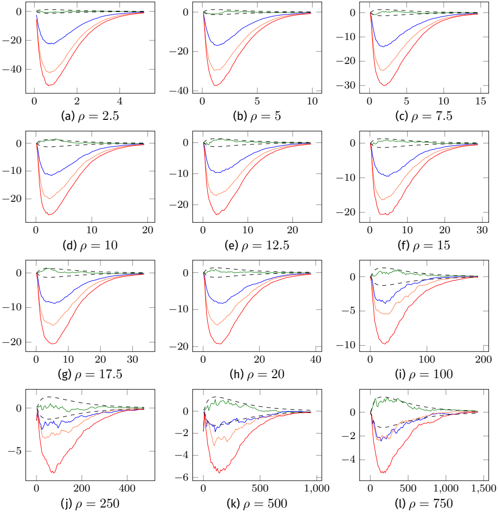
# Benchmark test Absorbing



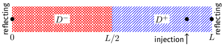

$t \to \sqrt{N}$(Emp. dist. of exit time − True dist.)

| | |
|---|---|
| SBM | Green |
| Uffink | Blue |
| HMYLA | Coral |
| SBMlin | Red |

$\rho = \frac{D_-}{D_+}$, $L = 2$, $x_0 = 0.1$, $dt = 0.001$, $N = 2\text{x}10^6$



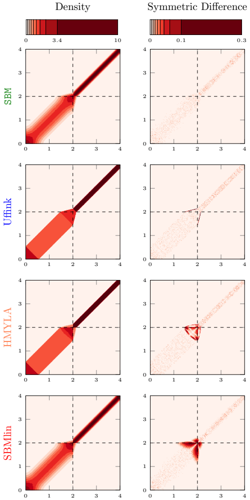
# Benchmark test SYMMETRY



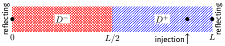

Density $q(t, x, y)$ (left) and $q(t, x, y) - q(t, y, x)$ (right) after 1 step.

| | |
|---|---|
| SBM | Green |
| Uffink | Blue |
| HMYLA | Coral |
| SBMlin | Red |

$\rho = \frac{D_-}{D_+} = 15$, $L = 4$, $dt = 0.01$, $N = 2x10^6$, starting points $(i + 1/2) * L/200$



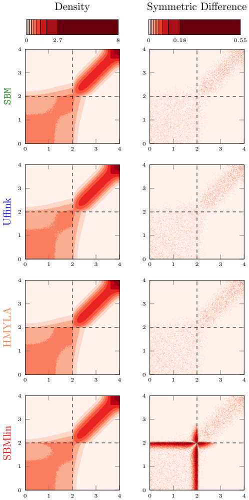
# Benchmark test SYMMETRY




Density $\mathfrak{q}(t, x, y)$ (left) and $\mathfrak{q}(t, x, y) - \mathfrak{q}(t, y, x)$ (right) after 20 steps.

| | |
|---|---|
| SBM | Green |
| HMYLA | Coral |
| Uffink | Blue |
| SBMlin | Red |

$\rho = \frac{D_-}{D_+} = 15$,
$L = 4$, $dt = 0.01$,
$N = 2x10^6$, $T = 0.2$,
starting points
$(i + 1/2) * L/200$



## Conclusion

- We have tested 4 methods on several benchmark tests, 2 relying on Gaussian type steps, and 2 on Uniform type steps.
- SBMlin failed all the tests!
- `SBM`, `HYMLA`, `Uffink` show adequate results in **steady state regime**.
- In **transient regime**, `SBM` $\geqslant$ `Uffink` $\geqslant$ `HYMLA`.
- Exit time are overestimated with `Uffink` and `HYMLA`.
- The lack of preservation of symmetry may explain the failure of SBMlin which however introduce less approximation than HYMLA.

> Symmetry $\Longrightarrow$ preservation of mass transfer
> A good scheme shall keep this physical property.

TODO

- Packaging the `sbm` library (APP registration, July 2018).
- New scheme for diffusion + convection (Preprint hal-01806465)
- Applying it to other schemes.

# Thanks a lot for your attention!

*Workshop* Validation approaches for multiscale porous media models

Nottingham, July 16, 2018